Heptanedioic acid

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 332 °C

Global applicability domain: Outside

Local applicability domain index: 6.83e-01

Confidence level: 5.44e-01

Nearest Neighbors from the Training Set

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Heptanedioic acid
Measured: 342
Predicted: 332

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Octanedioic acid
Measured: 346
Predicted: 332

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Hexanedioic acid
Measured: 338
Predicted: 330

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3-Ethyl-3-methylglutaric acid
Measured: 261
Predicted: 286

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Pentanedioic acid
Measured: 303
Predicted: 310